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Trimodal Random-Field Ising Systems in a Transverse Field

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Trimodal random-field Ising systems in a transverse field

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Abstract

The trimodal random-field Ising model with the presence of a transverse field is investigated by introducing a parameter p to simulate the fraction of spins not exposed to the external longitudinal magnetic field. Phase diagrams are obtained for different cases and conditions for the occurence of tricritical and reentrant phenomena are found. The competing effects on phase transitions due to the magnetic randomness and quantum fluctuations are also discussed.

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I. Introduction

The random-field Ising model (RFIM) has been a subject of extensive investigation in recent years,[1-3] because it helps simulate many interesting but complicated problems. A dilute uniaxial two-sublattice antiferromagnet in a uniform magnetic field fits this model in that random local fields couple linearly to the antiferromagentic order parameter.[4] It can also be used to describe such processes as the phase separation of a two-component fluid mixture in porous material or gelatine and the solution of hydrogen in metallic alloys.[5]

Of more interest is the random field effect on the structure of the phase diagram. The phase diagram may exhibit a tricritical point in the mean-field approximation (MFA). Since the correlation between spins is completely ignored in the MFA, it is not possible to discuss the dependence of the phase diagram on local structures. Various methods of approximation have been proposed to improve the results of the MFA in this model.[6,7] A pair approximation[8] which takes into account the local structure of the interaction pattern of the underlying system has been discussed within the RFIM, and phase diagrams are obtained for various coordination numbers.

The bimodal random-field Ising spin system in a transverse field has recently been discussed.[9] A method involving both the pair approximation and the discrete path-integral representation (DPIR)[10,11] has also been developed to treat this complicated problem.[12] Phase diagrams have been investigated, and conditions for the appearance of tricritical and reentrant phenomena have been examined.

As the form of the random-field distribution plays an important role in the determination of the order of phase transitions, we consider in this report the trimodal RFIM in a transverse field. Since the trimodal

distribution simulates a system in which a fraction p of the spins are not exposed to the external longitudinal field, it reduces the magnetic randomness in the system. The transverse field, on the other hand, gives rise to possible spin-flip transitions and hence works against the ordering. Our aim is to investigate the competing effects on the phase diagram from the magnetic randomness and the quantum fluctuations due to the transverse field.

II. Theory

For an Ising spin system in a transverse field with random fields h_i, the total Hamiltonian is given by

$$H = J \sum_{i,j} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^z - \Gamma \sum_i \sigma_i^x \quad , \tag{1}$$

where σ_i^x and σ_i^z are Puali matrices associated with the i-th site, Γ represents the uniform transverse field energy, and the random field is assumed to be a trimodal distribution of the probability[13]

$$P(h_i) = p\delta(h_i) + \frac{1}{2}(1-p)[\delta(h_i-h_o) + \delta(h_i+h_o)] \tag{2}$$

with the parameter p measuring the fraction of spins in the sample not exposed to the longitudinal magnetic field. The summation in the first term of (1) is taken over every pair of spins only once.

As discussed in Ref. 12, the problem can be treated in three steps. The Hamiltonian (1) is first written in the pair approximation in which the interacting system is replaced by a pair of spins in an effective field due to the spins at all other sites. The next step is to apply the DPIR in which the

effective pair Hamiltonian is split up into a reference part of a one-body Hamiltonian plus a two-body interaction. By expressing the single-spin effective field in terms of a two-spin effective field, the third step is to write down a single-spin effective Hamiltonian.

The standard procedure then leads to the single-spin mean free energy

$$
\begin{aligned}
-\beta\langle f(h_{eff})\rangle_h = {} & zp\ln\{2\cosh(\beta\sqrt{h_{eff}^2 + \Gamma^2})\} \\
& + (1-z)p\ln[2\cosh(\beta\sqrt{(\tfrac{z}{z-1}\,h_{eff})^2 + \Gamma^2})] \\
& + \tfrac{z}{2}(1-p)[\ln\{2\cosh(\beta\sqrt{(h_o+h_{eff})^2 + \Gamma^2})\} \\
& + \ln\{2\cosh(\beta\sqrt{(-h_o+h_{eff})^2 + \Gamma^2})\}] \\
& - \tfrac{1-z}{2}(1-p)[\ln\{2\cosh(\beta\sqrt{(h_o + \tfrac{z}{z-1}\,h_{eff})^2 + \Gamma^2})\} \\
& + \ln\{2\cosh(\beta\sqrt{(-h_o + \tfrac{z}{z-1}\,h_{eff})^2 + \Gamma^2})\}] + \tfrac{z\beta J}{2}\left\{\frac{p\,h_{eff}}{\sqrt{(h_{eff})^2 + \Gamma^2}}\right. \\
& \times \tanh(\beta\sqrt{h_{eff}^2 + \Gamma^2}) - \frac{1-p}{2}\left[\frac{h_o + h_{eff}}{\sqrt{(h_o+h_{eff})^2 + \Gamma^2}}\right. \\
& \times \tanh(\beta\sqrt{(h_o+h_{eff})^2 + \Gamma^2}) + \frac{-h_o + h_{eff}}{\sqrt{(-h_o+h_{eff})^2 + \Gamma^2}} \\
& \left.\left.\times \tanh(\beta\sqrt{(-h_o+h_{eff})^2 + \Gamma^2})\right]\right\}^2 , \qquad (3)
\end{aligned}
$$

where z is the coordination number, h_{eff} is the effective field in the pair approximation, $H_{eff} = \frac{z}{z-1} h_{eff}$ is the single-spin effective field, and the symbol $\langle \ldots \rangle_h$ stands for the average over the random field distribution. When the average free energy is expanded in terms of h_{eff}, second-order transition lines can be determined from the zero point of the coefficient of the second-order term in Eq. (3). Thus when the average free energy in Eq. (3) is expanded into a power series of h_{eff}, we find

$$\frac{p}{G} \tanh(G/t) + (1-p) \left\{ \frac{G^2}{\left[G^2+H^2\right]^{3/2}} \tanh(\sqrt{G^2+H^2}/t) \right.$$

$$\left. + \frac{H^2}{t(G^2+H^2)} \operatorname{sech}^2(\sqrt{G^2+H^2}/t) \right\} = \frac{z}{z-1} \quad , \tag{4}$$

where we have defined the dimensionless parameters

$$t = 1/\beta zJ \quad , \qquad G = \Gamma/zJ \quad , \qquad H = h_o/zJ \quad . \tag{5}$$

Phase diagrams can be calculated from Eq. (4) and the results reduce to those for the case of a bimodal random-field distribution discussed in Ref. 12 when $p = 0$.

Let us now look at various limiting cases. In the absence of random fields, the system is described by the TIM which is a special case corresponding to $p = 1$. It then follows from (4) that the second-order phase transition is determined by

$$\frac{1}{G} \tanh(G/t) = \frac{z}{z-1} \quad . \tag{6}$$

For $T_c = 0$ K, Eq. (6) implies a critical transverse field

$$\Gamma_c = (z-1)J \quad . \tag{7}$$

This is in excellent agreement with the numerical results obtained from series expansion for different coordination numbers.[14,15]

When the transverse field is absent, the model reduces to a trimodal RFIM. The second-order phase transition line follows by setting $G = 0$ in Eq. (4). Thus, we have

$$(1-p)\tanh^2(H/t) = 1 - \frac{zt}{z-1} \tag{8}$$

By expanding the average free enrgy in Eq. (3), we find from the fourth-order term in h_{eff} that the tricritical points are given by

$$(1-p)[1-\tanh^2(H/t)][1-3\tanh^2(H/t)] + p = 0 \quad . \tag{9}$$

It is not difficult to show that in the limit $z \to \infty$, the MFA results are recovered as expected.

In general, when the trimodal random fields and the transverse field are both present, the condition for the existence of tricritical points can be obtained in the limit $t \to 0$ in the following manner.[16] We expand the free energy (3) in terms of the effective field h_{eff}, and then set the coefficients of the second- and fourth-order terms in the expansion to zero separately. The resulting coupled equations are

$$p/G_o + (1-p)\, G_o^2/(G_o^2 + H^2)^{3/2} = z/(z-1) \tag{10}$$

$$p/G^5 + (1-p)(G_o^2-4H^2)/(G_o^2+H^2)^{7/2} = 0 \quad . \tag{11}$$

The tricritical point can be determined unambiguously from Eqs. (10) and (11). We first eliminate H from these equations and then solve for the critical transverse field, which can be expressed as a $G_o(p,z)$. The tricritical points can exist when $G < G_o$ and disappear when $G \geq G_o$. The function G_o is calculated numerically for some particular cases, and the results are plotted in Fig. 1. In addition, our numerical study shows that the phase transition remains to be second order for all temperatrue down to 0 K, where $0.22 \leq p \leq 1$. These results indicate that the appearance of tricritical phenomena is suppressed by either the increasing quantum effects due to the transverse field or by the increased dilution of the random field distribution.

III. Phase diagrams

Phase diagrams of the trimodal RFIM in a transverse field are determined numerically in the tH-plane from Eq. (4) for various cases. Results are presented in three groups corresponding to the transverse fields G = 0.45, 0.6 and 0.72. Each group contains three cases with the parameter p chosen to be 0.05, 0.1 and 0.25. In every case, calculations are carried out for the simple cubic structure, hexagon close-packed structure and mean-field approximation, with the corresponding coordination number z = 6, 12 and ∞, respectively.

It is observed from Figs. 2(a) and 2(b) that the tricritical point exists in every case considered because $p < 0.22$ and $G < G_o$ are both satisfied. There is, however, no tricritical point for either of the three cases in Fig. 2(c) in which p = 0.25. On the other hand, the phase transitions exhibit reentry within small ranges of the H-value as tricritical

points disappear, indicating possible competition between randomness and quantum fluctuations.

Figure 3 shows the phase diagrams for G = 6. According to the curve b of Fig. 1, $G > G_o$ over the whole range of p for z = 6 for which no tricritical point can exist. This is indeed the case, as can be clearly seen from the figure. Curve 1 for all the three p-values calculated does not exhibit any tricritical point, but the reentrant phenomenon occurs within a certain range of H, which decreases with increasing p. When p = 0.25, as in Fig. 3(c), no more reentry can be observed.

In Fig. 4, we plot the phase diagrams for G = 0.72, which is larger than G_o for any z according to Fig. 1. Thus one can only see reentrant phenomena when the parameter p is small. In Fig. 4(c) in which p = 0.25, the second-order phase transition lines for all three z-values extend through the whole range of H.

In conclusion, we have calculated phase diagrams for the trimodal random field Ising model in a transverse field. The third peak introduced in addition to the bimodal distribution of random field simulates cases in which the distribution of nonmagnetic-like impurities or spins not exposed to the longitudinal magnetic field. Its presence reduces the randomness of the system and competes with the quantum flluctuations due to the trnasverse field. We have shown the existence of the critical transverse field G_o above which the tricritical point can no longer occur. For the parameter p, we find that the system may exhibit tricritical transition only when $p < 0.22$, instead of 0.25 predicted by the MFA.

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Figure captions

1. Variation of the critical reduced transverse field G_o with the parameter p for different coordination numbers. (a) $z = 4$, (b) $z = 6$, (c) $z = 12$, (d) $z = \infty$.
2. Phase diagrams for $G = 0.45$. Curves 1, 2, 3 correspond to $z = 6$, 12, ∞, respectively. The paramter p is (a) 0.05, (b) 0.1 and (c) 0.25.
3. Same as in Fig. 2, except $G = 0.6$.
4. Same as in Fig. 2, except $G = 0.72$.

Fig. 1

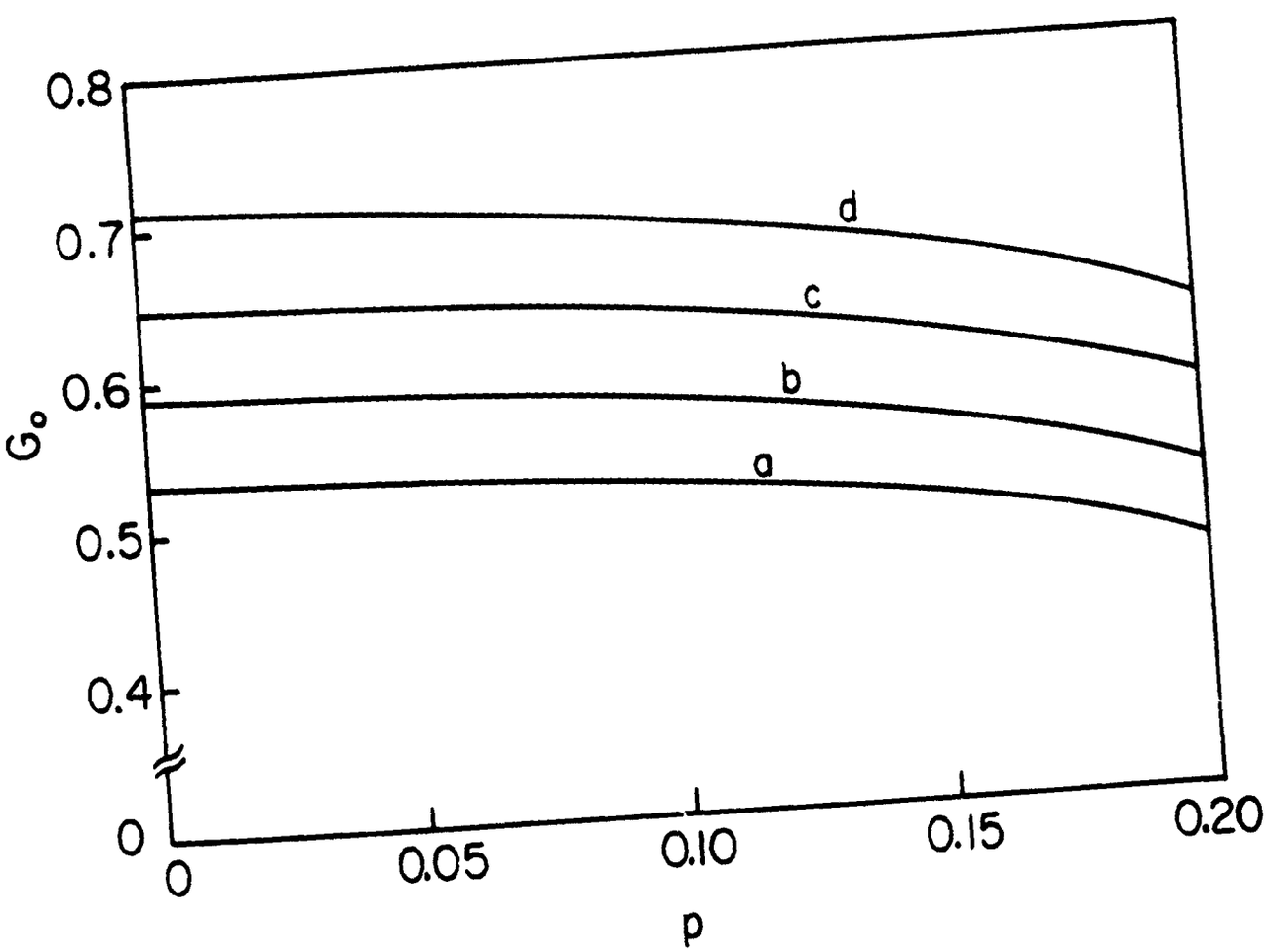

Fig. 2

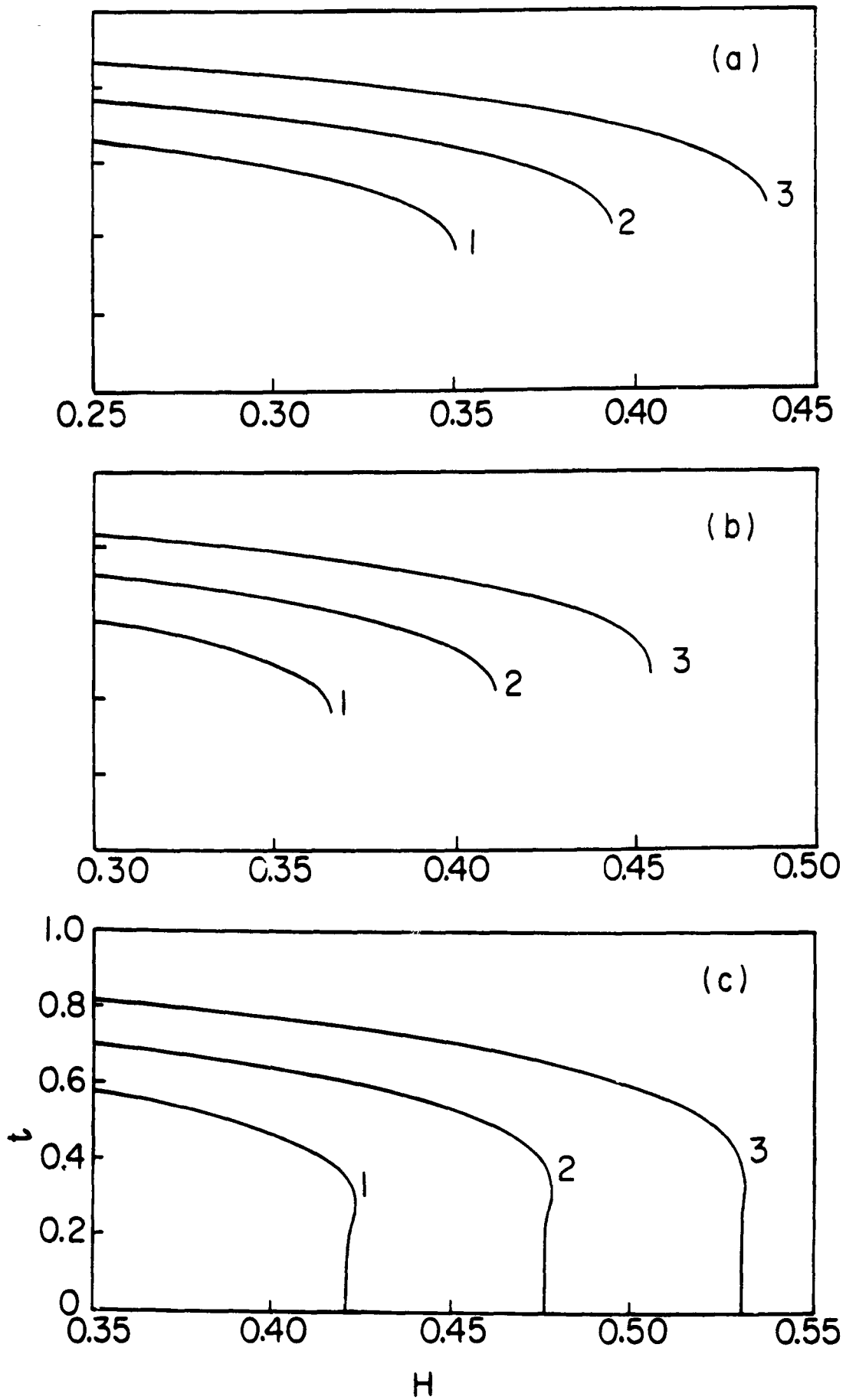
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Fig. 3

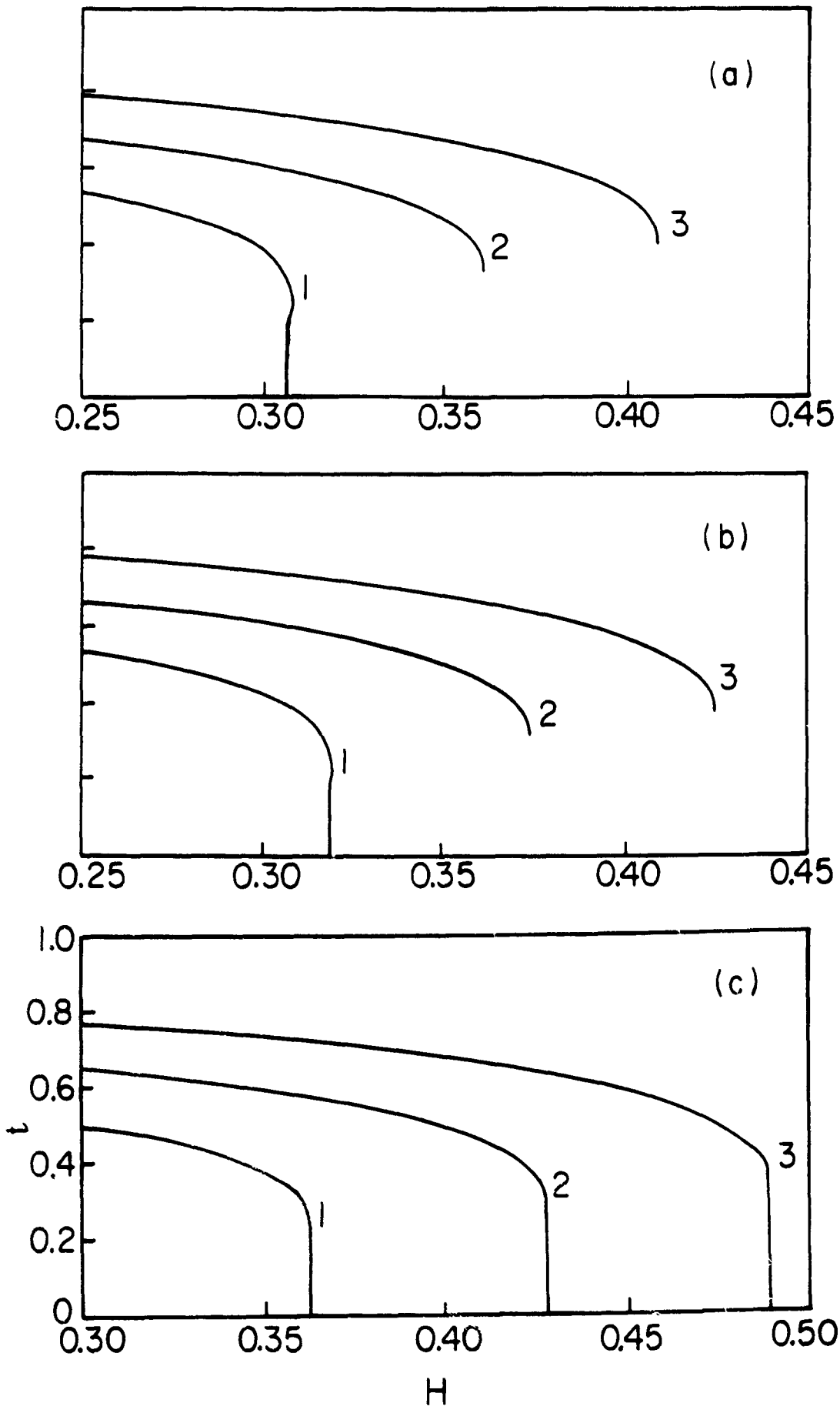
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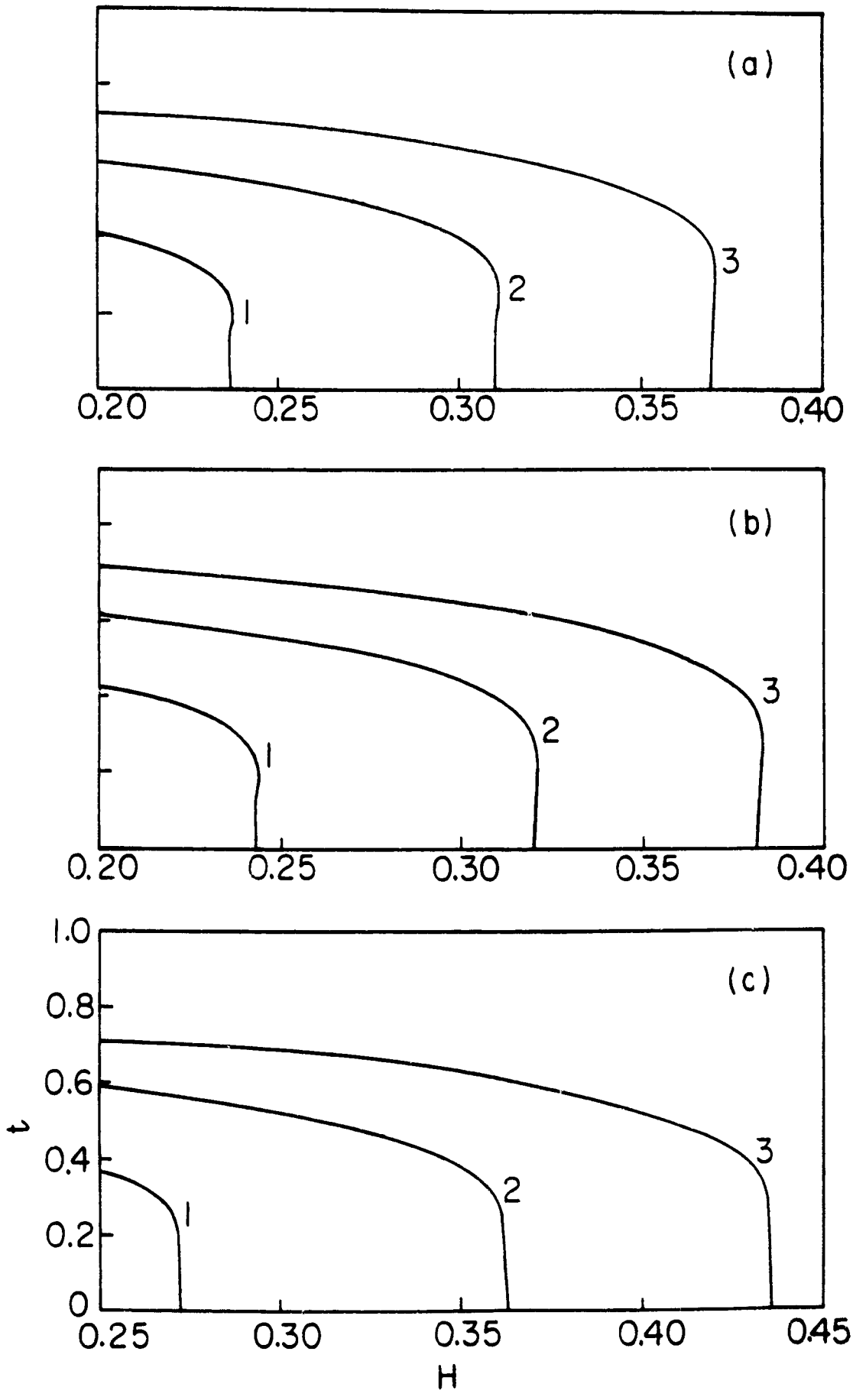
Fig. 4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